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Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding

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Published in:
Journal of the American Chemical Society

DOI:
[10.1021/ja062389h](https://doi.org/10.1021/ja062389h)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2006

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Rodriguez-Docampo, Z., Pascu, S. I., Kubik, S., & Otto, S. (2006). Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding. *Journal of the American Chemical Society*, 128(34). <https://doi.org/10.1021/ja062389h>

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SUPPORTING INFORMATION

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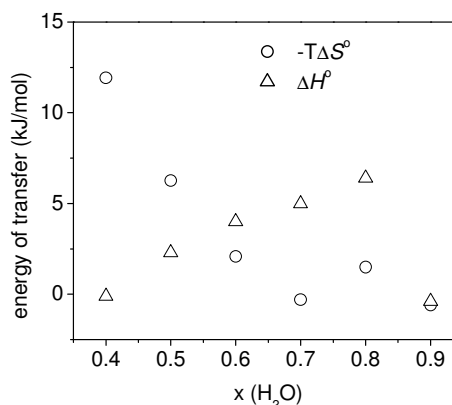
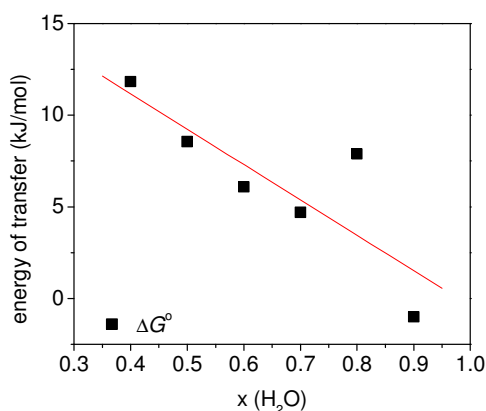
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Transfer thermodynamics of iodide anion from water to water + acetonitrile

Data taken from: Hefter, G.; Marcus, Y.; Waghorne, W.E. *Chem. Rev.* **2002**, *102*, 2773-2836.

x an (%)		from Table 42	at 298.15K	from Table 40	
	x H ₂ O	ΔS_t° (J mol ⁻¹ K ⁻¹)	$T\Delta S_t^\circ$ (kJ mol ⁻¹)	ΔH_t° (kJ mol ⁻¹)	ΔG_t° (kJ mol ⁻¹)
5	0.95			-3.4	
10	0.9	2	0.596	-0.4	-0.996
20	0.8	-5	-1.491	6.4	7.891
30	0.7	1	0.298	5	4.702
40	0.6	-7	-2.087	4	6.087
50	0.5	-21	-6.261	2.3	8.561
60	0.4	-40	-11.926	-0.1	11.826
70	0.3	-43	-12.820	-3.7	9.120
80	0.2	-40	-11.926	-8.7	3.226
90	0.1			-11	
100	0	-88	-26.237	-9.3	16.937



Linear fit of data for ΔG_t° : $\Delta G_t^\circ = -19 \times \text{mol fraction}(\text{H}_2\text{O}) + 19$

So for an increase in the mol fraction of water by 0.1 the ΔG_t° from water to a water-acetonitrile mixture becomes less unfavorable by 1.9 kJ/mol. Thus, desolvating iodide becomes 1.9 kJ/mol more costly for every 0.1 increase in the mol fraction of water.